



***Integrity ★ Service ★ Excellence***

# **Low Density Materials**

**Date: 03 07 2013**

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**Program Officer**

**AFOSR/RTD**

**Air Force Research Laboratory**

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# 2013 AFOSR SPRING REVIEW



NAME: **Low Density Materials**

## PORTFOLIO DESCRIPTION :

Transformative research targeting advanced materials that enable substantial reductions in system weight with enhancements in performance and function.

***INCREASING SPECIFIC PERFORMANCE***  
**(performance/pound)**

## PORTFOLIO SUB-AREAS:

Structural Lightweighting



Multifunctionality



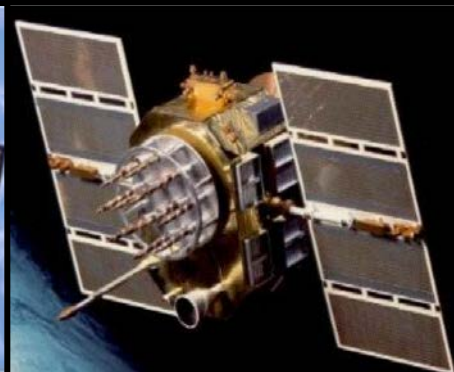
Materials By Design



Increased emphasis on forging interdisciplinary teams to address broad-base challenges



# Why Low Density Materials?



*If it has **structure** and **ris**es above the ground, material density is important!*



*Material density impacts: **payload capacity, range, cost, agility, survivability, environmental impact....***





# Research Thrusts

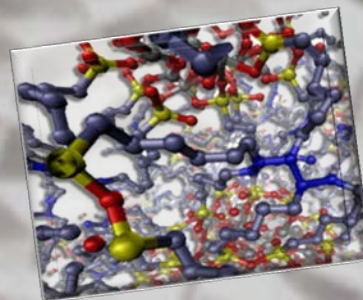
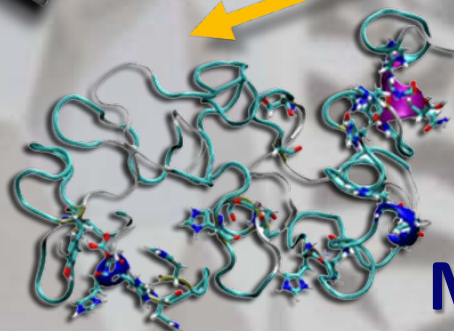
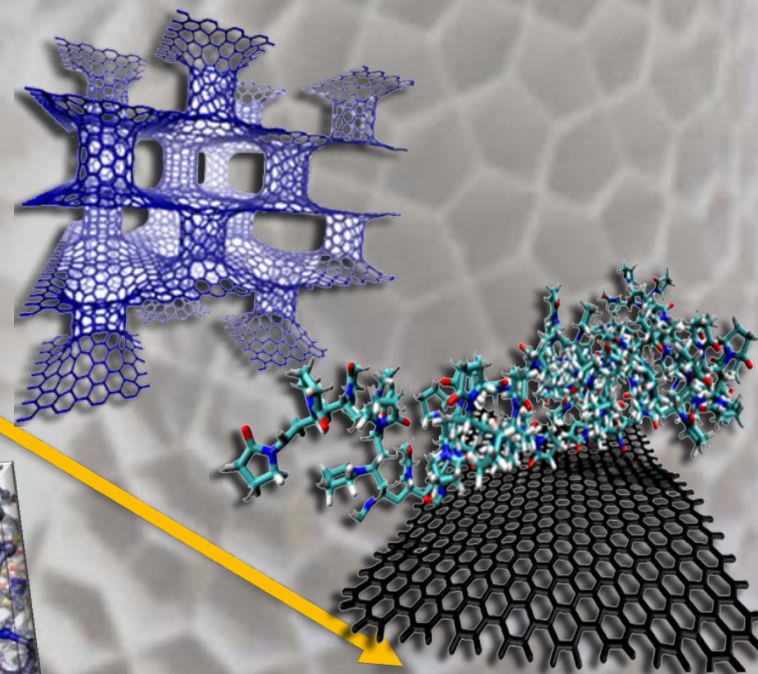
## STRUCTURAL LIGHTWEIGHTING

*- taking the weight out of traditional composites*



## MULTIFUNCTIONALITY

*- coupling structure + function*



## MATERIALS BY DESIGN

*- bottoms-up materials design based on structural requirements*



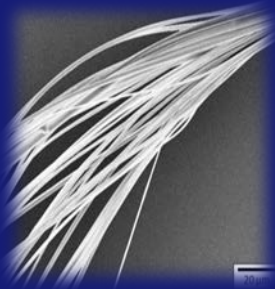
# Structural Lightweighting Highlights



## Nanomaterials for Aerospace Structures

Translating the revolutionary properties of nanostructured materials to macroscale load-bearing structures

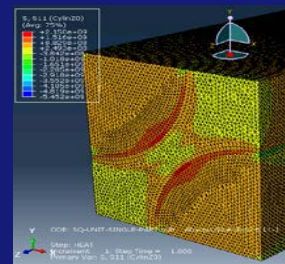
- Signed Memorandum of Agreement with NASA LaRC
- Nanotube Assemblages for Structures Workshop, April 2012
- Established working group to develop coordinated interagency roadmap for structural nanomaterials



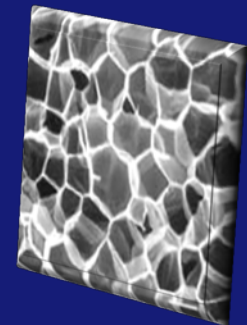
Improved Fibers  
& Resins



Nanotechnology



Predictive Modeling



Nanoscale  
Porosity



# Materials By Design



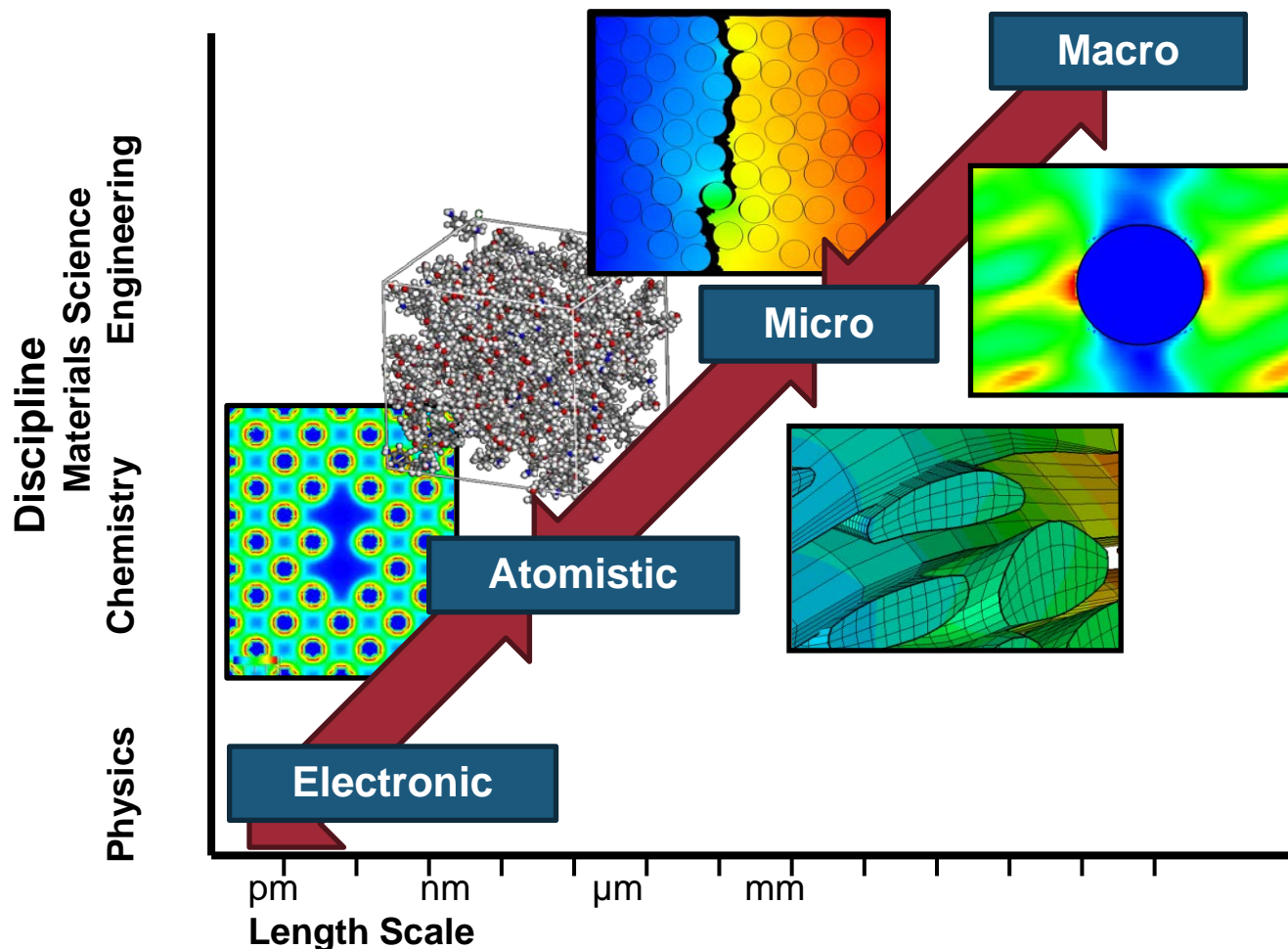
**Design the structure  
based on limitations of  
the material**

**Design the material  
based on structural  
requirements**





# Connecting Atomistic & Microscale Behavior -- Essential for Materials Design



Dr. Tim Breitman  
AFRL/RXBC



Dr. Rajiv Berry  
AFRL/RXBN



Prof. Jim Moller





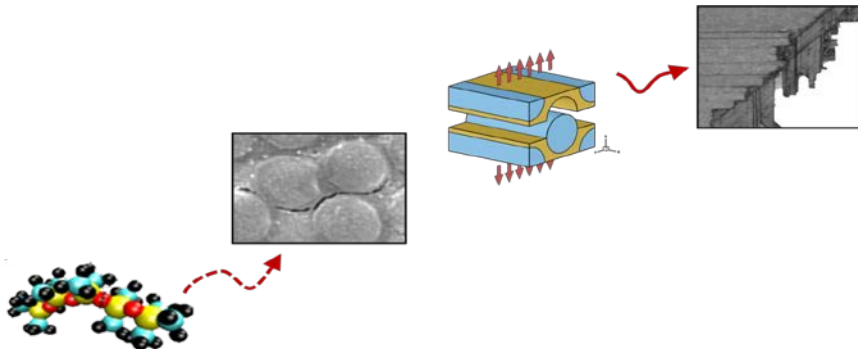


# Connecting Atomistic & Microscale Behavior -- Essential for Materials Design



## Goals

- Derive resin fracture toughness from atomistic behavior
- Integrate atomic & molecular simulation methods into materials system analysis

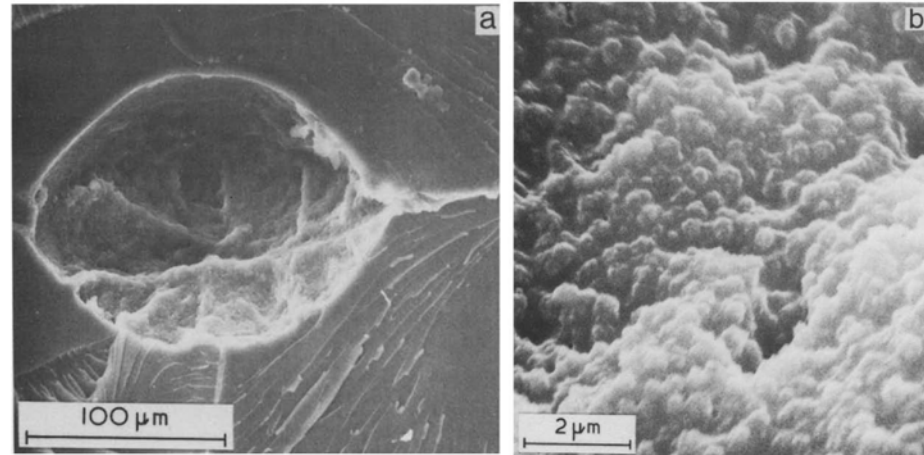


## Limits - Current Practice

- Unrealistic methods used to represent strain rate
- Bond scission not considered or permitted via a force field parameterized for other contexts
- Toughness properties in continuum scale based on empiricism

## Fundamental Scientific Challenges

- No direct knowledge of fracture nucleation



(Morgan, Mones, Steele, Polymer, 1982)

## Novel Approach

- Strain-rate-controlled deformation
- Bond scission in covalently-bonded glassy polymer systems via Quantum Mechanics
- Detailed post-processing

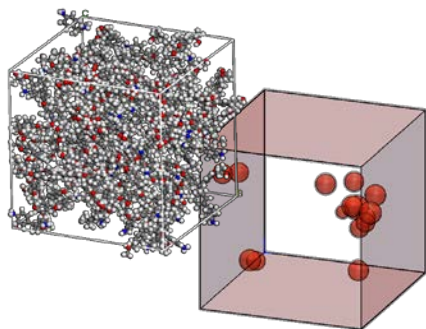


# Integrated Quantum Mechanics-based Bond Scission with Molecular Dynamics



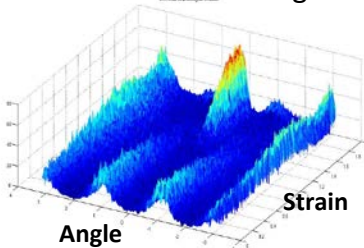
## Technical Approach

- Quantum mechanical (QM) simulation of highly-strained zones
- Bond scission during deformation
- Unique analysis of molecular re-conformation dynamics & free volume development



Free volume clusters in molecular system

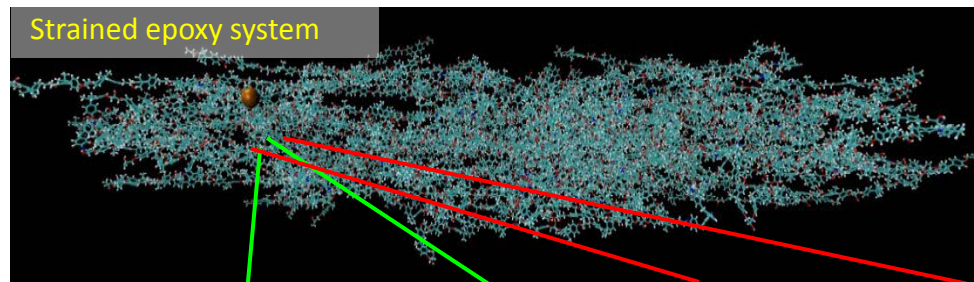
Chain backbone dihedral angle associated to uncoiling



## Impact

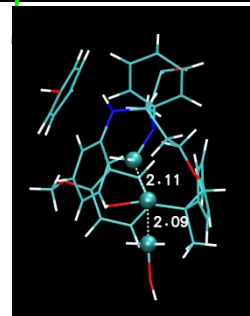
- Improved understanding of the origins of fracture: captured subatomic, molecular, & nanoscale events at nucleation.
- Effect of resin formulation on nucleation.
- Information for micro-mechanics

## Accomplishments

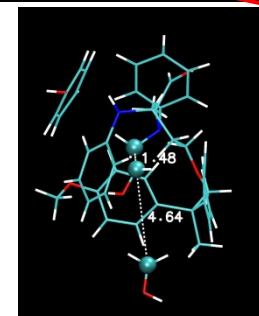


Strained epoxy system

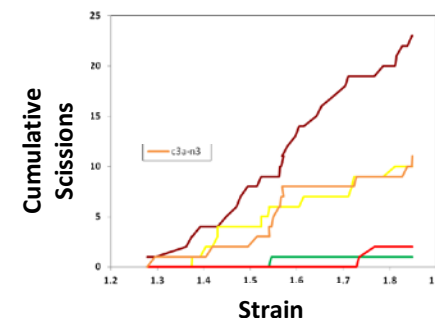
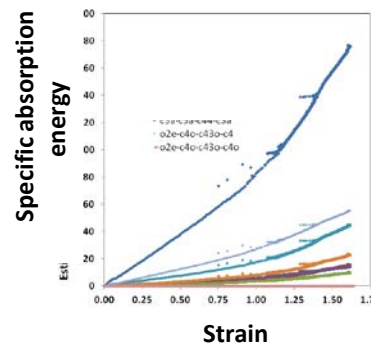
Before Scission



After Scission



Segments of molecular network absorbing mechanical energy



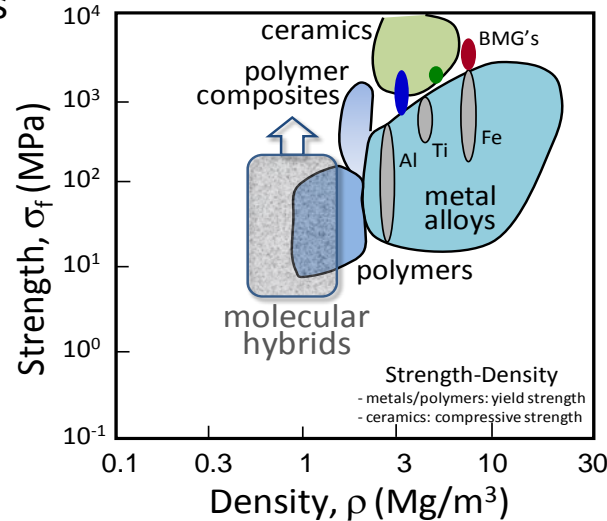
Weak points of the cross-linked network



# Molecular Design of Hybrid Materials

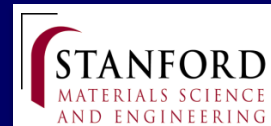


- Molecular hybrids exhibit the lowest densities with the potential for significant increases in strength and toughness properties
- Organic and inorganic components from molecular to macro length scales enables mechanically-robust materials with multifunctional property sets
- Opportunity to tailor mechanical, thermal, electrical, and optical properties

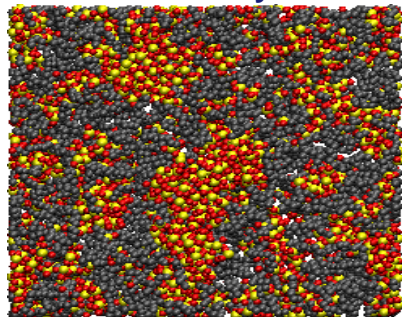


Prof. Reinhold Dauskardt

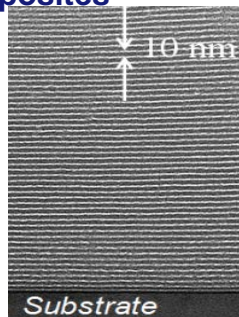
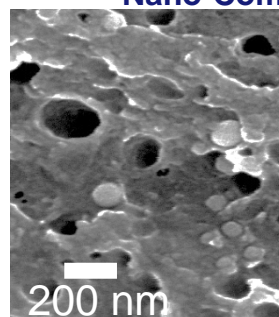
- Fellow of ACerS and ASM
- Recipient of Maso, IBM, SIA, and TMS Awards for fundamental contributions to structural and electronic materials



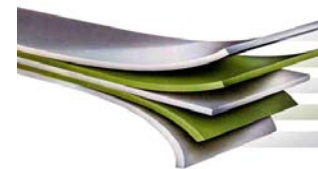
**Molecular Hybrids**



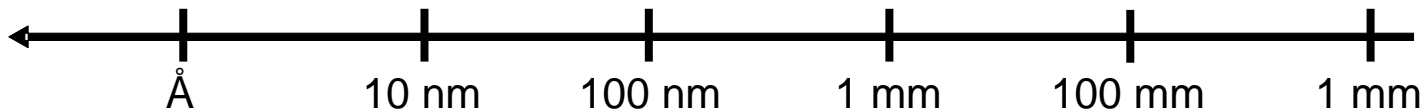
**Porous Hybrids and Nano-Composites**



**Hybrid Laminates**



**Multifunctional Devices**



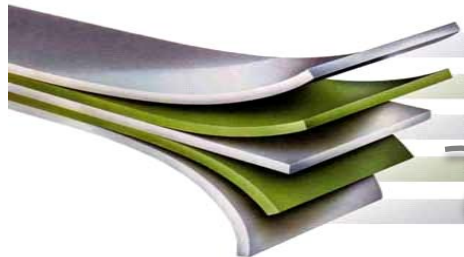
**Bottom-Up Design of Multifunctional Hybrid Materials**



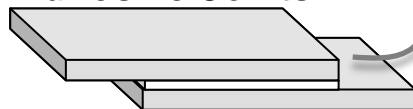


# Molecular Hybrid Design: High Performance Bonding

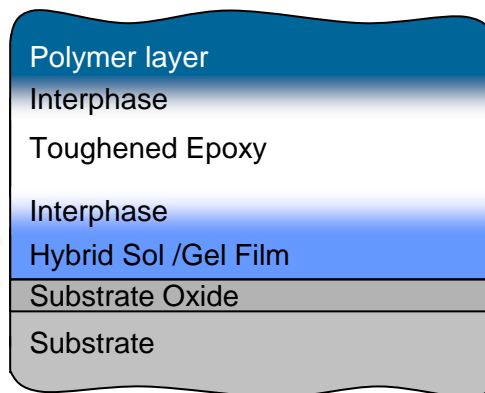
Performance Laminates



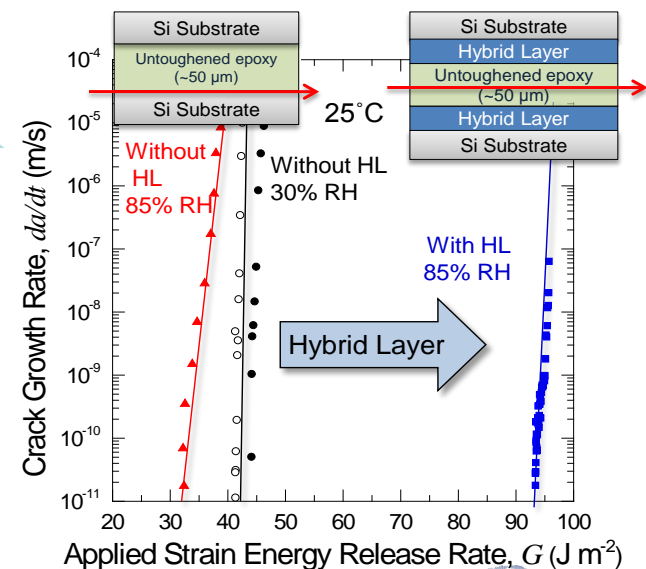
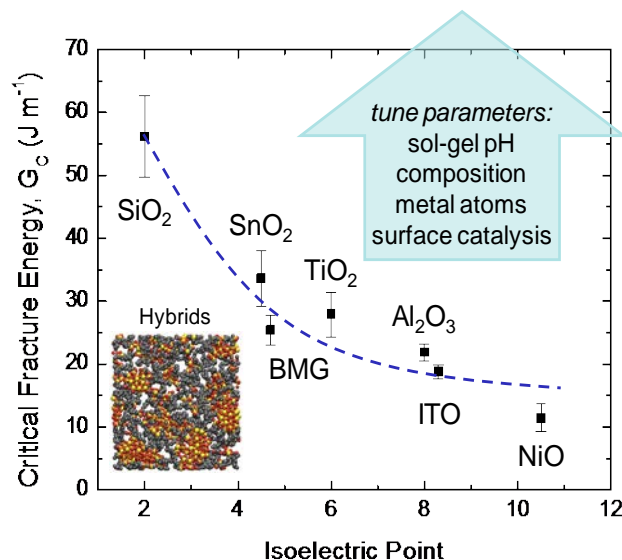
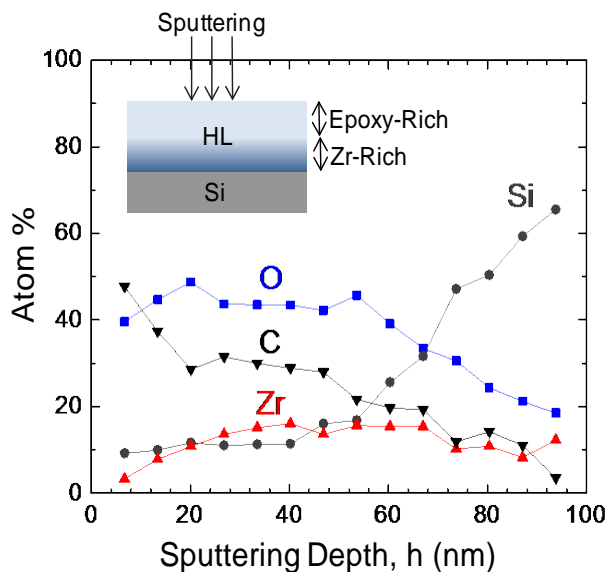
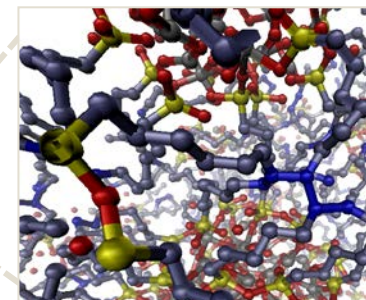
Adhesive Joints



Interphase Region



Hybrid Molecular  
Hybrid Sol / Gel Layers

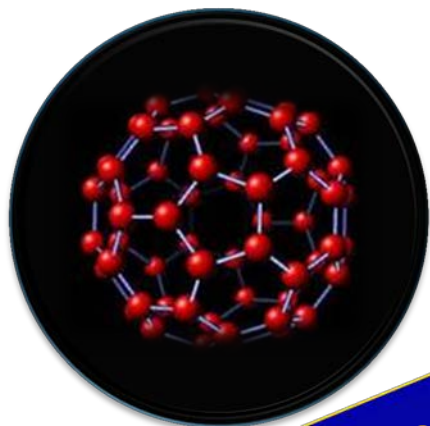




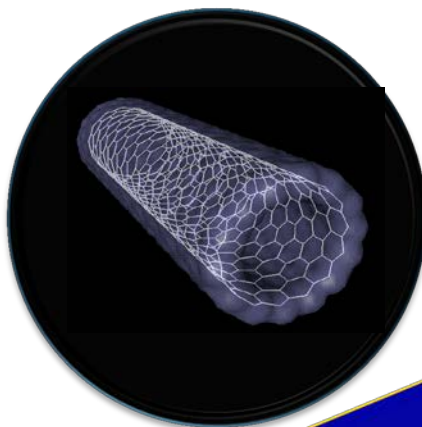


# Nanostructured Carbon

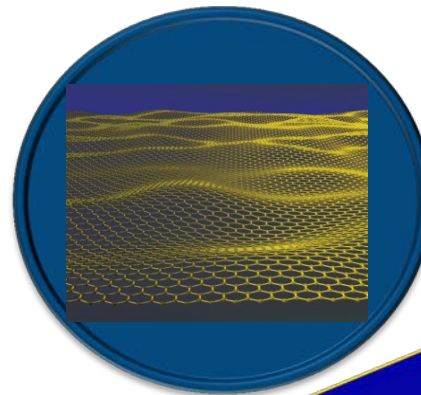
0D  
Fullerene



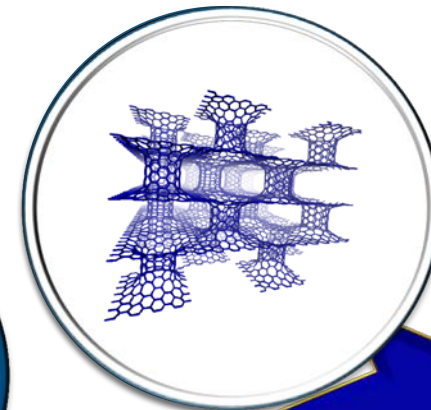
1D  
Carbon  
Nanotubes



2D  
Graphene



3D



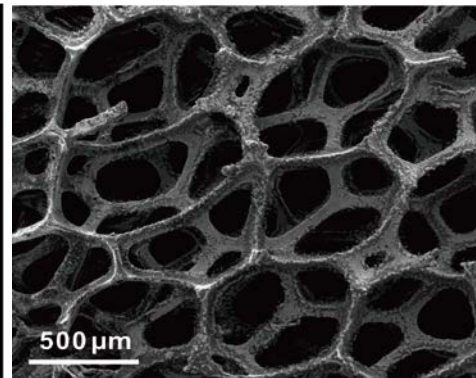
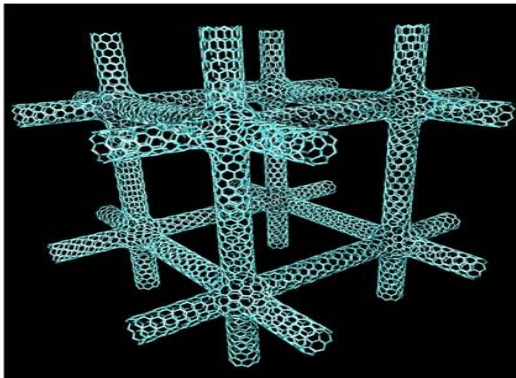
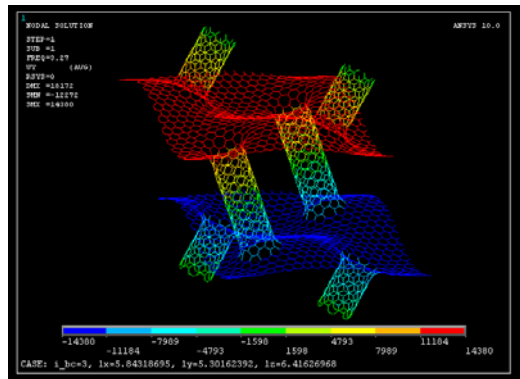
1985

1991

2004



# MURI 11: Nanofabrication of 3D Nanotube Architectures



## Overarching Scientific Challenges

- Covalent junctions between building blocks leading to 3D networks
- Systematic characterization/modeling of the junctions and properties
- Development of scalable growth processes for 3D nanostructured solids
- Structure-property correlations of mechanical and transport properties

## Potential Payoffs

- Translation of exceptional 1D and 2D properties of tubes and sheets to 3D
- High surface area for energy storage and conversion devices
- Orthogonal transport of phonons for thermal management
- Mechanical reinforcement



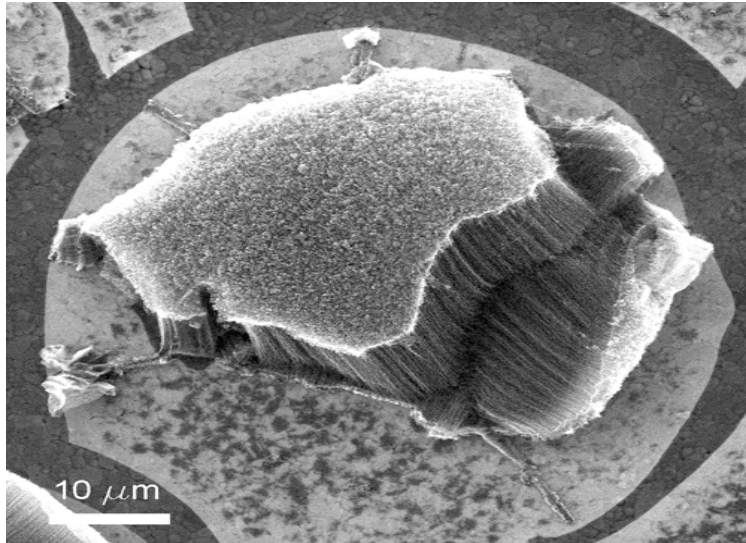
# Rice U. MURI Team 2012 Highlights



## Towers of nanotubes sprout from graphene

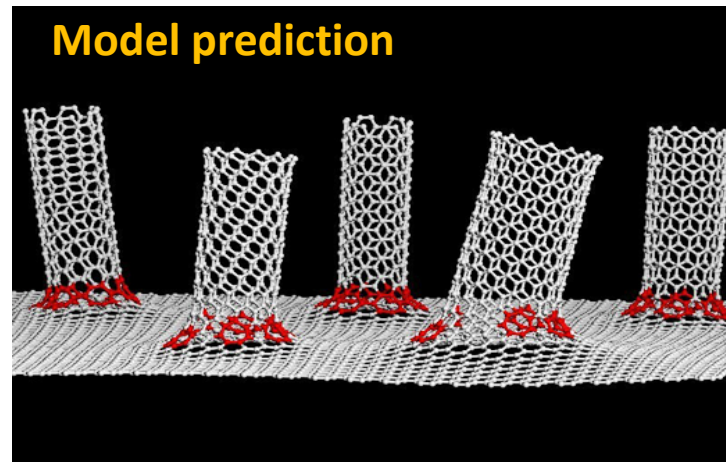
(Futurity, Sci. and Technology, Nov. 27, 2012.)

(Nature Communications, 3:1225 doi: 10.1038/2234 (2012))

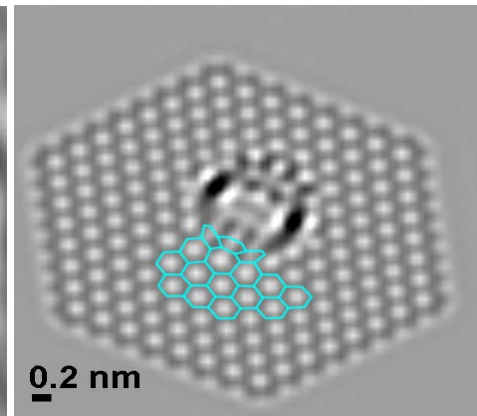
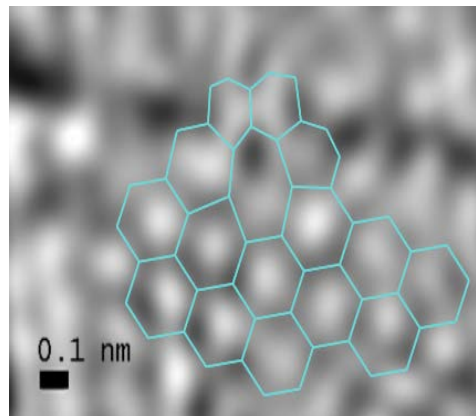


Surface area > 2,000 m<sup>2</sup>/gm

Comparison of simulated and experimental STEM images illustrating covalent bonding between CNTs and graphene



7-atom rings at the graphene-nanotube junction creates a seamless conductor



Prof. James Tour



Prof. Boris Yakobson





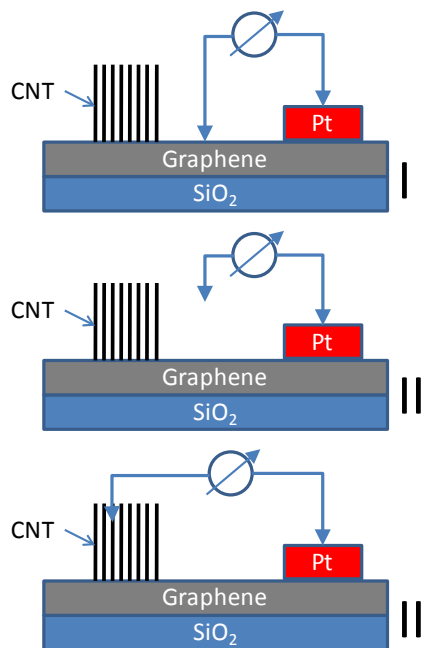
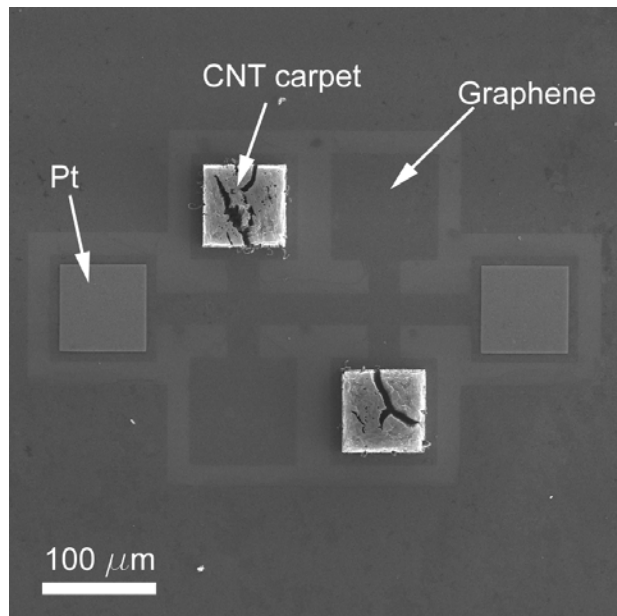


# Rice U. MURI Team 2012 Highlights

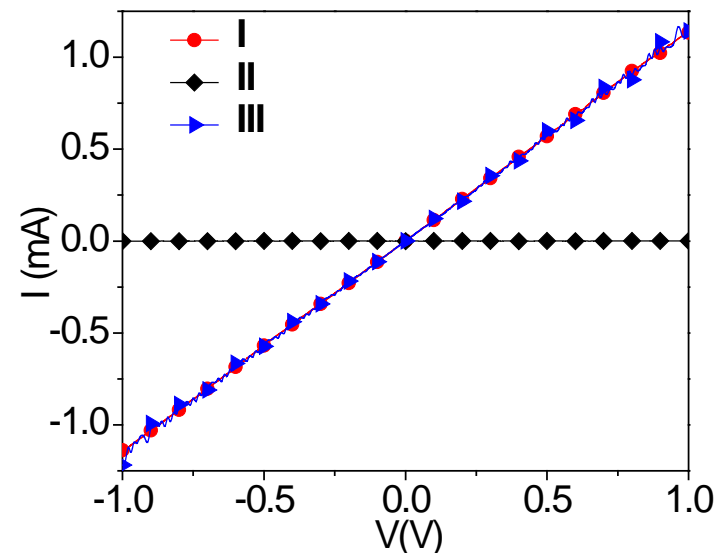


## Electrical properties of the 3D CNT/graphene nanostructures

(Nature Communications, 3:1225 doi: 10.1038/2234 (2012))



### Ohmic contact at CNT and graphene junctions







# Rice U. MURI Team 2012 Highlights



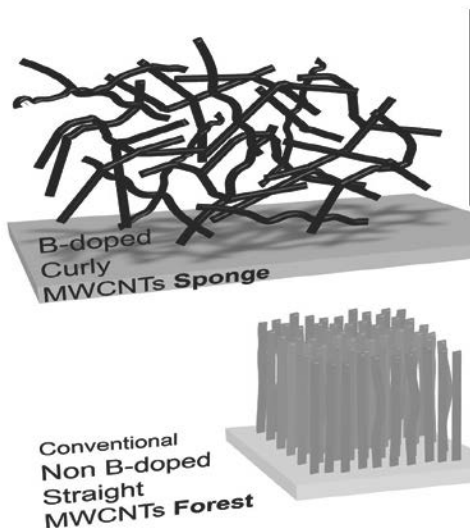
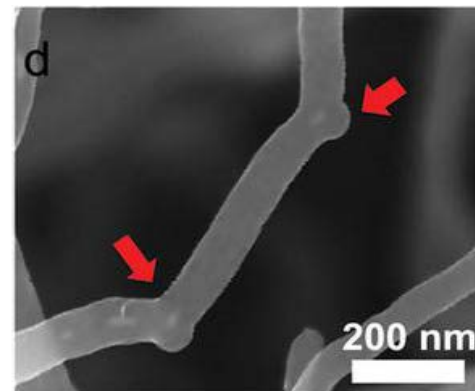
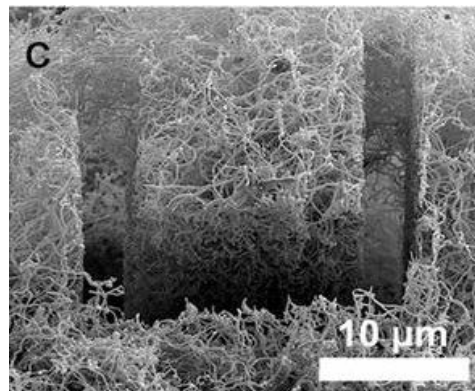
## 3D Solids of Boron-Doped Nanotube Networks (CBxMWNT sponges)



Prof. P. Ajayan  
Rice Univ.



Prof. Mauricio  
Terrones  
Penn State Univ.

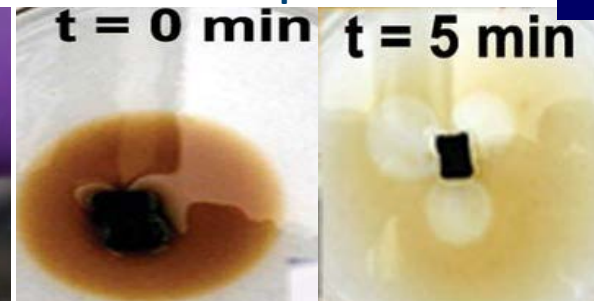


Covalent  
junctions  
established  
via boron  
doping led  
to novel  
properties

Hydrophobic



Oleophilic





# MURI Discovery Leads to Tech Transition



## Carbon Sponge Solutions, Inc. - Road to commercialization

**Nanotube sponge soaks up oil**

RiceUniversity ☒ Subscribed 443 videos



**NANOTUBE SPONGE ABSORBS OIL**  
Rice University

0:09 / 2:49

61,952

Published on Apr 17, 2012 by [RiceUniversity](#)

A sponge made of pure carbon nanotubes with a dash of boron shows remarkable ability to absorb oil spills from the surface of water.

285 likes, 2 dislikes

CSS, Inc. is a spin-off company out of Rice University (Houston, TX) founded in August 2012 (by student Daniel Hashim) with a mission to research, develop, and manufacture patent protected 3-D nanosponge products from the lab to the marketplace. Exploiting the nanomaterial's unique combination of multifunctional properties at both the nano-scale and macro-scale, many possible applications are expected for the environment, energy, and biomedical industries.

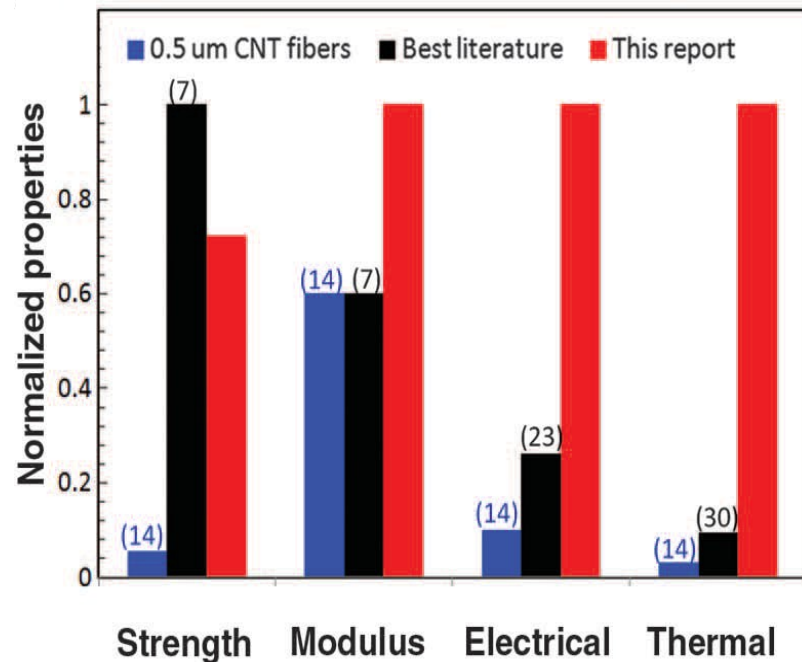


# CNT Fiber Tech Transition



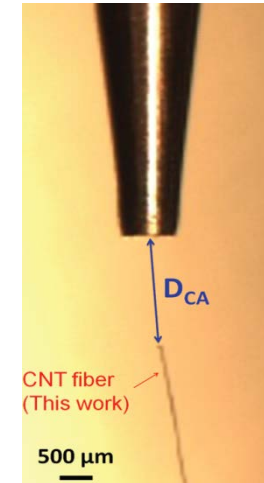
*“...high-performance multifunctional carbon nanotube (CNT) fibers that combine the **specific strength, stiffness, and thermal conductivity of carbon fibers** with the **specific electrical conductivity of metals**. ”*

(Science, 11 January 2013: Vol. 339 no. 6116 pp. 182-186.)

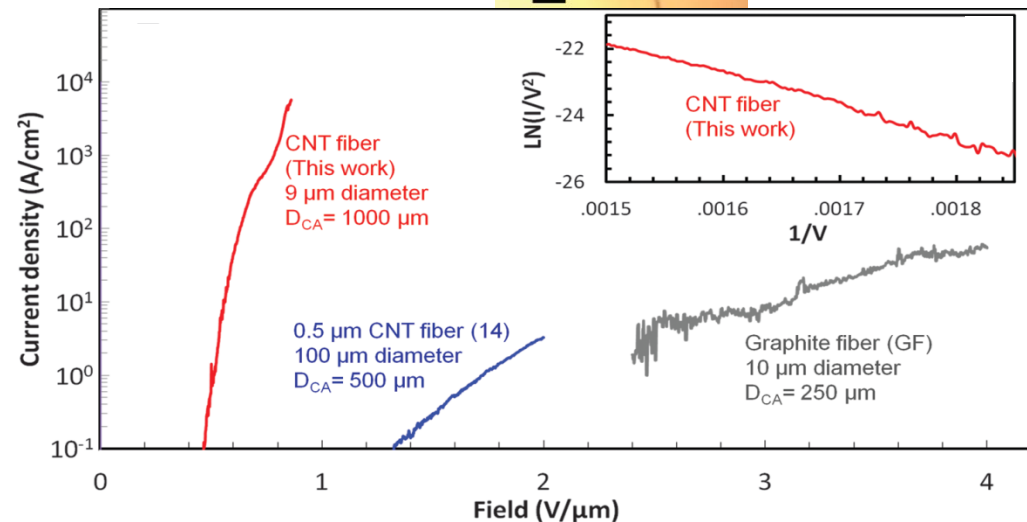


**Tech Transition**  
- AFRL/RX  
- Teijin Aramids

Field Emission Studies



Prof. Matteo Pasquali





# Basic Research Initiative

## AFOSR/NSF Joint Research Solicitation

### ODISSEI: Origami Design for Integration of Self-assembling Systems for Engineering Innovation

**Advance understanding of folding and unfolding of materials structures across scales for design of engineered systems**

**Jointly reviewed and funded 8 grants totaling approx. \$16M**

- **Synthesizing Complex Structures from Programmable Self-Folding Active Materials**, Richard Malak, Texas A&M U.
- **Mechanical Meta-Materials from Self-Folding Polymer Sheets**, Christian Santangelo, U. of Massachusetts Amherst
- **Photo-Origami**, Hang (Jerry) Qi, U. of Colorado at Boulder
- **Externally-Triggered Origami of Responsive Polymer Sheets**, Jan Genzer, North Carolina State U.
- **Programmable Origami for Integration of Self-assembling Systems in Engineered Structures**, Daniela Rus, Massachusetts Institute of Technology
- **Multi-field Responsive Origami Structures - Advancing the Emerging Frontier of Active Compliant Mechanisms**, Mary Frecker, Pennsylvania State U.
- **Uniting Principles of Folding and Compliant Mechanisms to Create Engineering Systems**, Larry Howell, Brigham Young U.
- **Multi-scale Origami for Novel Photonics, Energy Conversion**, Max Shtein, U. of Michigan Ann Arbor







# Joint RX, RQ Labtask

## Adaptive Origami for Efficiently Folded Structures

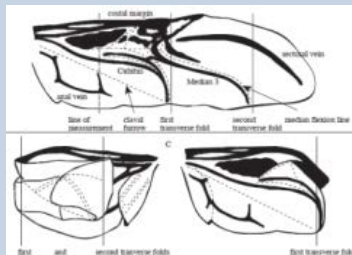
### STRUCTURES

#### Aeronautics

Light and strong



Origami Honeycomb

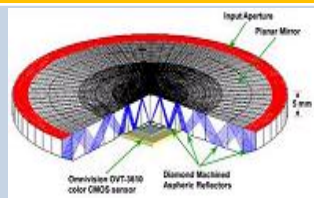


Wing folding

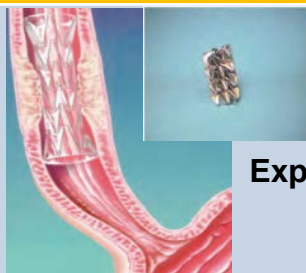


Shock absorbing structures

#### Optics, Sensors, Energy Harvesting, Bio



Ultrathin, High-Resolution Origami Lens



Solar origami

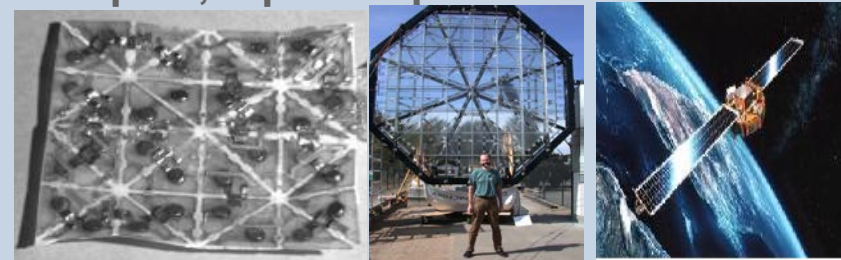
Expandable stents



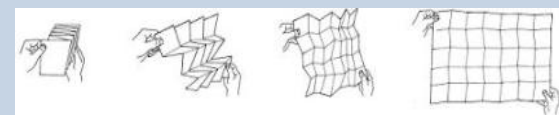
### MECHANISMS

#### Aerospace

Compact, repeated pattern

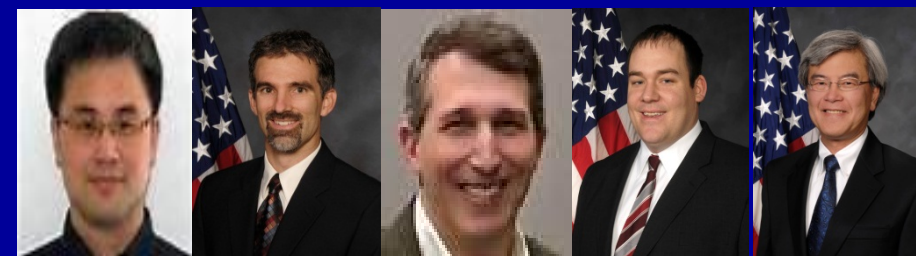


Self folding sheet



Deployable Solar sails, Antennas

#### Research Team



James Joo



Greg Reich



Rich Vaia



Tim White



Loon-Seng Tan

<http://www.origami-resource-center.com/origami-science.html>

DISTRIBUTION STATEMENT A – Unclassified, Unlimited Distribution





# Research Community Leadership



## AFOSR Low Density Materials

### AFRL

#### DIRECTORATES

RX, RV, RQ, RW  
LRIRs, STTRs,  
MURIs,  
Workshops,  
Reviews, Visits

#### INTERNATIONAL

US-India Tunable  
Materials Forum

US-AFRICA  
Initiative

### DOD COMMUNITY

Reliance 21 Board  
Materials and  
Processing COI

### OTHER AGENCIES



Lightweight  
Structures



Nanostructured  
Materials



Origami  
2D Beyond Graphene



# Acknowledgements



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Northeastern U.



Markus Buehler  
MIT



Satish Kumar  
Georgia Tech



Yuris Dzenis  
U. Nebraska



Greg Odegard  
Michigan Tech



Samit Roy  
U. Alabama



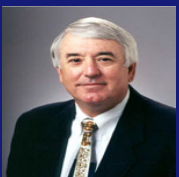
Ajit Roy  
AFRL/RX



Brandon Arritt  
AFRL/RV



Benji Marayama  
AFRL/RX



Frank Harris  
U. Akon



Alex Zettyl  
UC Berkeley



Ben Wang  
Georgia Tech



Cheol Park  
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Stephen Cheng  
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Richard Liang  
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Ryan Justice  
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Chris Muratore  
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Ashlie Martini  
UC Merced



Jeff Youngblood  
Purdue U.



Robert Moon  
Forrest Products



Changhong Ke  
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Binghamton U.



Mesfin Tsige  
U. Akron



Rodney Priestley  
Princeton U.



Henry Sodano  
U. Florida



Micah Green  
Texas Tech U.



Soumya Patnaik  
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Rice U.



Liming Dai  
Case Western  
Reserve U.



Sharmila  
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Wright State U.



Olesya Zhupanska  
U. Iowa



James Seferis  
GloCal Network



Philip Bradford  
NC State U.



Yuntian Zhu  
NC State U.



# THANK YOU

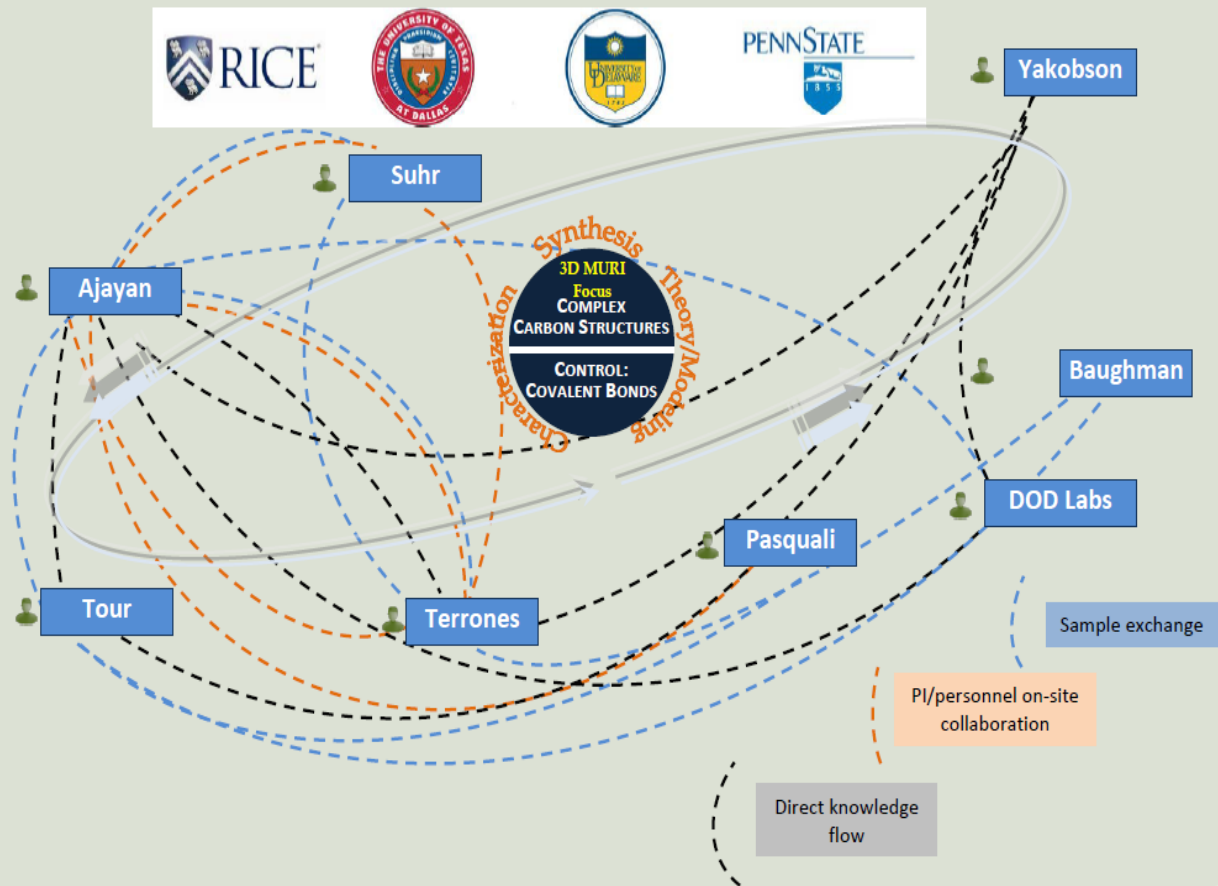




# Rice Univ. MURI Team: Strong Multidisciplinary Collaborations



3D-MURI Interaction Chart



Prof. Pulickel Ajayan, Lead PI  
Prof. James Tour  
Prof. Boris Yakobson  
Prof. Matteo Pasquali  
Rice Univ.

Prof. Mauricio Terrones  
Penn State Univ.

Prof. Ray Baughman  
Univ. Texas Dallas

Prof. Jonghwan Suhr  
Univ. Delaware

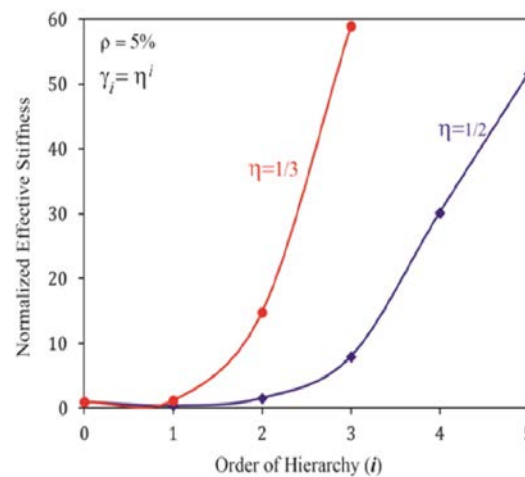
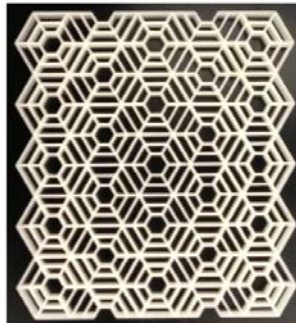
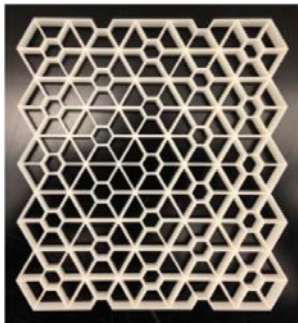
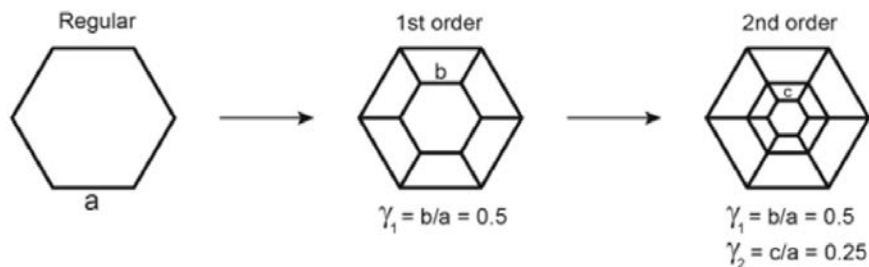


# Hierarchical Organization in Materials Design

## Goals

- Develop fundamental understanding of the role of hierarchy in controlling properties and functionality in material surfaces, interfaces and in cellular structures
- Analytical and predictive numerical models for studying the mechanical behavior of hierarchical honeycombs, composite lattice structures and bonded joints with non-flat interfaces

## Self-similar Hierarchical Spiderweb Honeycombs with 1<sup>st</sup> and 2<sup>nd</sup> order hierarchy



Numerical simulations show significant increase in the effective stiffness of spiderweb honeycombs compared to regular honeycombs of the same mass/density



Prof. Ashkan Vaziri,  
Northeastern Univ.  
• AFOSR YIP Award





# Increasing Specific Performance in Aerospace Platforms



A pyramid diagram with three horizontal layers, each containing text. The top layer is labeled "MATERIALS BY DESIGN", the middle layer is labeled "MULTIFUNCTIONALITY", and the bottom layer is labeled "STRUCTURAL LIGHTWEIGHTING". The pyramid is blue with yellow and orange borders.

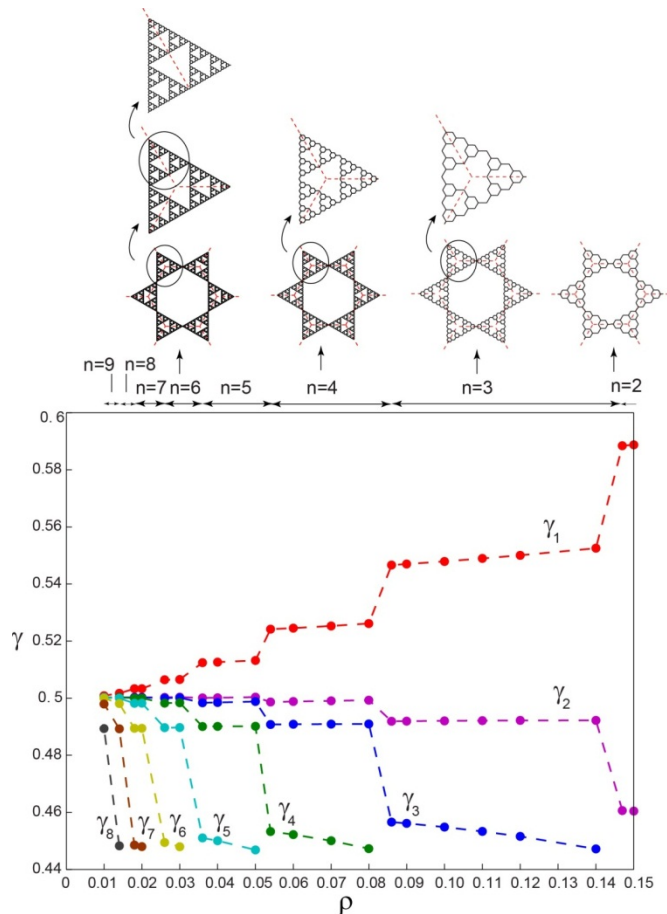
**MATERIALS  
BY DESIGN**

**MULTIFUNCTIONALITY**

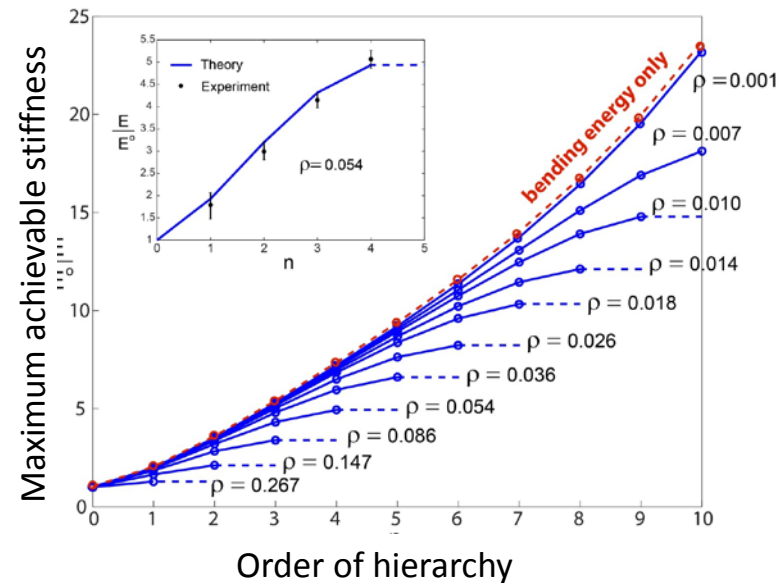
**STRUCTURAL LIGHTWEIGHTING**



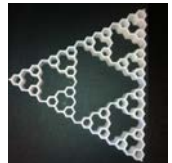
# Self-Similar Hierarchical Honeycombs



Optimum topology of hierarchical honeycombs, which approaches the fractal limit.



$n=3$



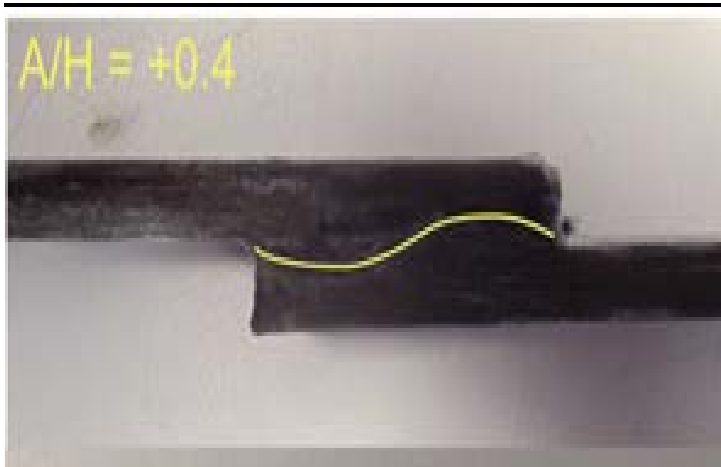
$n=4$

A new class of self-similar (fractal-appearing) hierarchical honeycombs with a wide range of elastic, plastic and load-induced expansion properties<sup>1</sup>

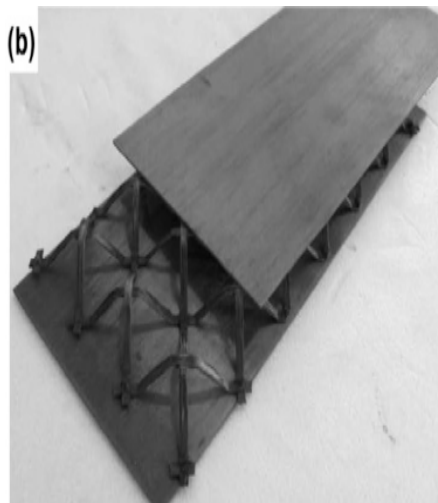
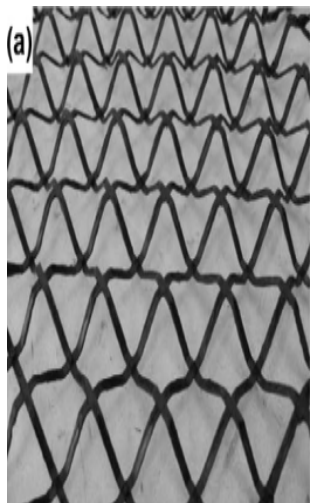
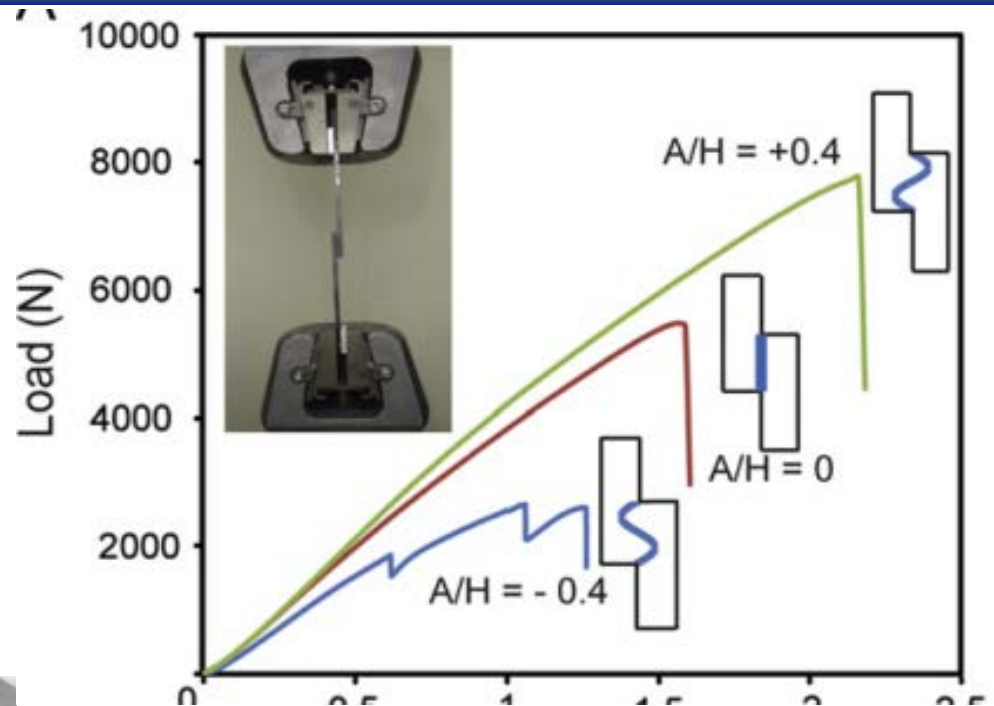




# Bioinspired Surface and Interfaces



Bonded joints with non-flat interface design.



Fiber reinforced composite panels with lattice cores